Bowing of the band gap pressure coefficient in $In_xGa_{1-x}N$ alloys

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The hydrostatic pressure dependence of photoluminescence, dE_{PL}/dp, of $In_xGa_{1-x}N$ epilayers has been measured in the full composition range $0<x<1$. Furthermore, *ab initio* calculations of the band gap pressure coefficient dE_G/dp were performed. Both the experimental dE_{PL}/dp values and calculated dE_G/dp results show pronounced bowing and we find that the pressure coefficients have a nearly constant value of about 25 meV/GPa for epilayers with $x>0.4$ and a relatively steep dependence for $x<0.4$. On the basis of the agreement of the observed PL pressure coefficient with our calculations, we confirm that band-to-band recombination processes are responsible for PL emission and that no localized states are involved. Moreover, the good agreement between the experimentally determined dE_{PL}/dp and the theoretical curve of dE_G/dp indicates that the hydrostatic pressure dependence of PL measurements can be used to quantify changes of the band gap of the InGaN ternary alloy under pressure, demonstrating that the disorder-related Stokes shift in InGaN does not induce a significant difference between dE_{PL}/dp and dE_G/dp. This information is highly relevant for the correct analysis of pressure measurements. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2837072]

I. INTRODUCTION

The $In_xGa_{1-x}N$ semiconductor alloy is of considerable importance for short and medium wavelength optoelectronics and photonics. InGaN is used for the construction of green-blue-violet light emitting diodes and blue-violet laser diodes.[1] Furthermore, InGaN-based solar cells[2] as well as detectors containing InGaN and operating in the short wavelength range[3] have been constructed in several laboratories. In spite of very advanced optoelectronic applications, mechanisms of radiative and nonradiative recombination in InGaN are still under debate. The discussion concentrates mainly on the Ga-rich range of InGaN ternary alloys. The pressure studies to be presented here, performed for $In_xGa_{1-x}N$ in the entire range $0<x<1$, can shed some light on the microscopic origin of recombination effects in InGaN alloys, enabling efficient light emission in a longer wavelength region, e.g., in the green range of the spectrum.

Usually, measurements of the photoluminescence (PL) energy E_{PL} under pressure are applied to determine dE_G/dp. Bulk crystals, thick epitaxial layers, or quantum structures are employed for such studies. However, there are particular effects that can lead to incorrect conclusions. We mention here three such situations. The first one concerns the involvement of a localized impurity/defect state in optical transitions responsible for PL. When the initial state of the optical transition is of localized nature, i.e., composed of wave functions from the entire Brillouin zone, its shift with pressure is much smaller than the upward shift of the conduction band minimum (CBM). Particularly in the case of a localized donor state we see that $dE_{PL}/dp \ll dE_G/dp$.[4] A second situation, in which $dE_{PL}/dp \ll dE_G/dp$, occurs for quantum structures built from wurtzite semiconductors from the nitride or ZnO family. In this case, pressure-induced changes of the internal electric field (caused by spontaneous and piezoelectric polarizations) cause a strong compensation of the opening of the band gap via the so-called quantum confined Stark effect. This mechanism was intensively studied during the last decade.[5–7] Third, a lowering of dE_{PL}/dp with respect to dE_G/dp occurs in the case of InN with large electron concentrations because of band filling effects in combination with the increase of the electron effective mass m^* with pressure.[8] This effect is only observable in InN because it has a narrow band gap and therefore a low, pressure-sensitive m^*.

In this work, we are interested in studies of the pressure dependence of the band gap in the entire range of ternary $In_xGa_{1-x}N$ $(0<x<1)$. Large Stokes shifts between E_G (from absorption/transmission measurements) and E_{PL} have been attributed to the presence of In-rich fluctuations in the InGaN region. PL probes these regions of locally reduced band gap of the alloy. Therefore, one may speculate that the pressure

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dependence of E_{PL} is sensitive to effects caused by In segregation. Investigation of this possibility is important for the interpretation of PL measurements on InGaN under hydrostatic pressure. From the experimental point of view, for corroboration of the usefulness of PL measurements for the determination of dE_G/dp, measurements of transmission/absorption of light or photoconductivity can be applied. Such experiments are technically more challenging than PL studies. Another method, used in the present work, to examine this involves theoretical predictions of the behavior of dE_G/dp calculated for InGaN alloys. Uniform and nonuniform arrangements of In cations in the GaN matrix are investigated in the modeling procedure in order to examine possible atom-distribution related effects. Theoretically calculated values of dE_G/dp will be compared with the measured dE_{PL}/dp.

The paper is organized as follows: after Sec. II, which contains descriptions of calculation procedures and experimental methods, in Sec. III theoretical and experimental results are presented. Section IV contains a discussion and our main conclusions.

II. METHODS

A. Theoretical procedures

The electronic structures of $In_xGa_{1-x}N$ alloys have been analyzed by *ab initio* calculations in a supercell geometry. The indium concentrations, $x=0.031$, 0.062, 0.124, 0.25, 0.50, and 0.75, were realized by substituting 1, 2, 4, 8, 16, and 24 Ga atoms, respectively, by In in a 64-atom supercell.

The calculations were performed in two steps using different approaches based on the local density approximation (LDA) to the density functional theory, with the Perdew-Zunger parametrization[9] of the Ceperley-Alder exchange-correlation.[10] We applied two computational schemes. The first one used pseudopotentials[11] as implemented in the Vienna *Ab initio* Simulation Package (VASP).[12] This code is well suited for calculations of the atomic relaxations in the whole supercell by minimizing the Hellman-Feynman forces. A cutoff energy of 30 Ry for the plane wave basis set was sufficient to obtain converged results. The *k*-space integrations were performed by summing over a $3\times3\times3$ mesh of Monkhorst-Pack special points.[13]

For each value of x and a given configuration of indium atoms, the relaxed atomic positions were determined. Then the $In_xGa_{1-x}N$ band structure was obtained by the second approach—the linear-muffin-tin-orbital (LMTO) method.[14] A full-potential (FP) version of the LMTO was applied.[15] The semi-core cation *d* states were included as local orbitals.[15] In fact, this was the main reason for choosing this method, because a proper inclusion of the coupling between the anion *p* and cation-semicore *d* is important for the accuracy of the calculated pressure coefficients (see below). So-called "empty spheres" (*E*) were included for the accuracy of interpolation of the charge density between the muffin-tin spheres at the sites of real atoms. No *E*-site orbitals were included. Although the LDA underestimates the band gaps of semiconductors, the pressure coefficients of the gaps are usually considered to be well described within this approximation.[16]

TABLE I. List of investigated $In_xGa_{1-x}N$ samples with In content x, thickness, and production source.

Sample	In content	Thickness (μm)	Grower
R335	0.13	1	Madrid[a]
R331	0.20	1	Madrid[a]
U368	0.72	0.41	Chiba[a]
U366	0.72	0.45	Chiba[a]
G925	0.37	1	FORTH[a]
G935	0.17	1	FORTH[a]
R594	0.58	0.35	Ritsumeikan[b]
R824	0.71	0.19	Ritsumeikan[b]
R810	0.80	0.2	Ritsumeikan[b]
R808	0.90	0.2	Ritsumeikan[b]
GS1366	0.89	0.25	Cornell[b]
GS1586	1	7.5	Cornell[c]

[a]Samples were examined in the context of the present work.
[b]Results were taken from Ref. 22.
[c]Results were taken from Ref. 8.

Theoretical calculations were performed for different configurations of In atoms inside the supercell, keeping the same overall concentration. No significant differences with regard to the resulting band gap pressure coefficients were found (see Sec. III), which indicates that clustering of In atoms does not influence the pressure behavior of the band gap. The calculations differ from Ref. 5 by the choice of a larger supercell (64 atoms instead of 32) and by detailed treatment of the lattice relaxation (not only the first neighbors, but all the atoms in the cell are relaxed). Also, the range of concentrations considered in this work is larger.

B. Experimental details

Pressure-dependent PL studies of $In_xGa_{1-x}N$ were perfomed on a range of samples from different laboratories: Universidad Politecnica de Madrid, Cornell University, FORTH Research Center in Heraklion, Ritsumeikan University, and Chiba University. In contents and thicknesses of the samples are summarized in Table I. Pressure-dependent measurements of the samples from Ritsumeikan and Cornell were already reported in previous publications (as indicated in the table). Data for these samples are also displayed in Table I. The variety of laboratories makes the results of our studies more general, since production-source-dependent effects are eliminated. As will be demonstrated, the full set of experimental data is coherent and exhibits a systematic trend in In content dependence.

All samples were grown by means of molecular-beam epitaxy on sapphire substrates, employing either an InN or a GaN buffer layer. The In contents reported in Table I were determined by means of x-ray diffraction. In the performed optical experiments, PL was excited by either the 325 nm line of a He-Cd laser (for $x<0.25$) or the 514.5 nm line of an argon laser (for $x>0.25$) and dispersed by a Spex 500 M monochromator. For detection purposes a GaAs-based photomultiplier tube with photon counting unit (for $x<0.25$) or a Ge-based photodiode (for $x>0.25$) were used. Hydrostatic pressures up to 10 GPa were applied by a diamond anvil cell (DAC) with argon as a pressure-transmitting medium, while

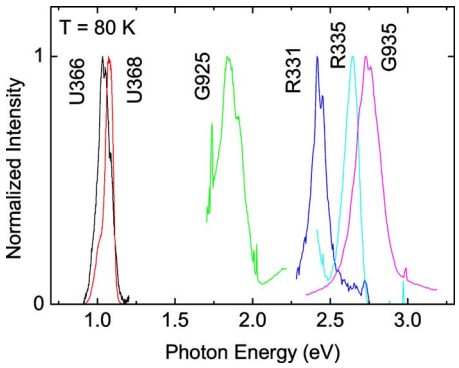

FIG. 1. (Color online) Normalized low-pressure spectra of the investigated $In_xGa_{1-x}N$ samples. In contents x are indicated. Displayed PL spectra were recorded at ambient pressure, except in the case of samples $G935$ ($x=0.17$) and $U368$ ($x=0.72$), for which PL was recorded at pressures of 0.50 and 0.57 GPa, respectively.

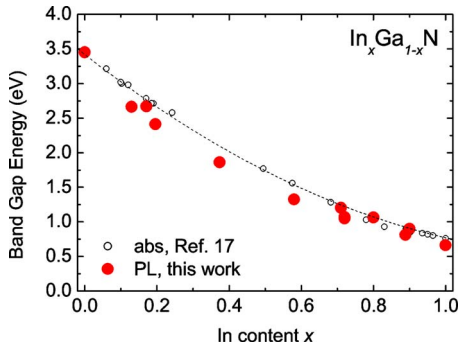

FIG. 2. (Color online) PL peak energy at ambient pressure and 80 K of the $In_xGa_{1-x}N$ samples investigated in the present work. In contents x are indicated. Also shown is the band gap energy dependence on In content as obtained via absorption measurements taken from Ref. 17. A fit of the band gap energies (using a bowing parameter of 1.43 eV) is indicated by a dashed line.

the pressure was calibrated by means of the $R1$-line of a ruby crystal. Pressure dependences of PL spectra were measured at a temperature of 80 K.

III. RESULTS

Normalized low-pressure PL spectra of the investigated samples, recorded at 80 K, are displayed in Fig. 1. The main trend is a redshift of the PL peak as the In content increases, which agrees with the expected lowering of the band gap energy. By "low-pressure" we denote the lowest hydrostatic pressure that could be realized experimentally inside the closed DAC. This pressure is occasionally slightly but not significantly above ambient pressure. This is due to the fact that samples are sometimes damaged on the full release of hydrostatic pressure at the end of the pressure cycle, which thwarts performing the PL measurement at ambient pressure. Using $In_xGa_{1-x}N$ samples with very different In contents, we are able to map the behavior of dE_{PL}/dp across the full range of ternary alloys from GaN to InN. Please note that the PL spectrum of the $In_xGa_{1-x}N$ sample with $x=0.13$ has a slightly lower PL peak energy than the sample with $x=0.17$, which is partly due to the fact that these PL spectra were recorded at different pressures (see figure caption). For the same reason there is a small difference between the peak energies of $U366$ and $U368$, for both of which $x=0.72$.

The PL peak energies of the complete set of investigated InGaN samples are plotted in Fig. 2 as a function of In content. For the discussion of the Stokes shift between PL and absorption edge, also shown are results concerning the band gap energy as obtained from absorption measurements. A fit of the band gap energies (using a bowing parameter of 1.43 eV) is indicated by a dashed line. Both absorption results and fit are taken from Ref. 17. It is seen that PL peak emissions have lower energies than the band gap energy for the full range of In contents. The Stokes shift tends to increase when the In content x approaches 0.5, i.e., when the distribution of Ga and In atoms is maximally randomized. This validates the supposition that the Stokes shift in InGaN is related to microstructural disorder. The observed Stokes shift is relevant for the discussion of pressure-dependent results below.

Hydrostatic pressure dependences of two selected samples, $U366$ and $R335$, are shown in Figs. 3(a) and 3(b), respectively. A blueshift of the PL peak with increasing pressure can be observed, in accordance with the opening of the band gap. Qualitatively similar results in terms of signal-to-noise ratio and range of applied pressures were obtained for the other investigated samples. Fabry-Perot oscillations, such as those observable for sample $U366$ in Fig. 3(a), were removed during analysis by means of Fourier filtering.

Dependences of PL peak energies on hydrostatic pressure are displayed for all investigated samples in Fig. 4. Also shown are linear fits of the PL pressure coefficient dE_{PL}/dp. The values obtained for dE_{PL}/dp in the case of $In_xGa_{1-x}N$ samples $U366$ ($x=0.72$), $U368$ ($x=0.72$), $G925$ ($x=0.37$), $R331$ ($x=0.20$), $G935$ ($x=0.17$), and $R335$ ($x=0.13$) are, respectively, 23.2, 24.1, 26.0, 28.3, 32.6, and 33.0 meV/GPa.

In Fig. 5, the dependence of the measured values of dE_{PL}/dp on In content is displayed graphically. The error bars are based on the data scatter in combination with experimental uncertainties. The experimental point concerning GaN is taken from Ref. 18. Also shown is the theoretical

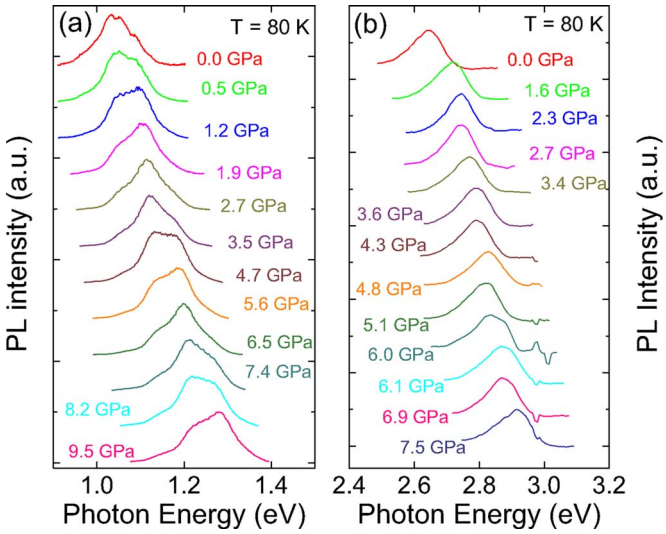

FIG. 3. (Color online) Hydrostatic pressure dependences of PL spectra of (a) sample $U366$ ($x=0.72$) and (b) sample $R335$ ($x=0.18$).

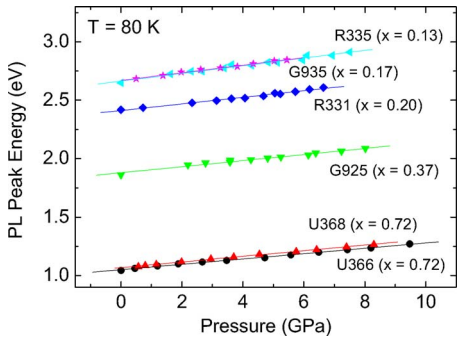

FIG. 4. (Color online) Hydrostatic pressure dependences of PL peak energies of all investigated $In_xGa_{1-x}N$ samples. In contents x are indicated. Linear fits of the PL pressure coefficient dE_{PL}/dp are indicated by solid lines.

dependence of dE_G/dp that resulted from the *ab initio* approach discussed in Sec. II A. Double theoretical points at $x=0.125$ and $x=0.5$ correspond to different configurations of In atoms in a supercell. Both experimental and theoretical results show pronounced bowing of the pressure coefficient, with a nearly constant value of about 25 meV/GPa for $In_xGa_{1-x}N$ epilayers with $x>0.4$ and a relatively steep dependence for $x<0.4$. A good agreement between experiment and theory is found. In the next section, we will discuss the implications of the obtained results.

IV. DISCUSSION AND CONCLUSIONS

The calculated values of dE_G/dp for the binaries GaN and InN in Fig. 5 are in agreement with earlier observations[19,20] and with the trends suggested by Wei and Zunger,[21] who predicted a weak decrease of dE_G/dp when the cation-atomic number increases. Their other prediction of a significant decrease of dE_G/dp when the anion atomic number decreases is also seen to be correct on comparing the values obtained here with typical dE_G/dp values of other members of the III–V family, which are in the range of 100–150 meV/GPa. In particular, the value of about 25 meV/GPa characterizing InN is the lowest among III–V semiconductors.

At this point it is worthwhile to mention that results of PL studies by Li *et al.*[19] of InN and $In_{0.5}Ga_{0.5}N$ as a function

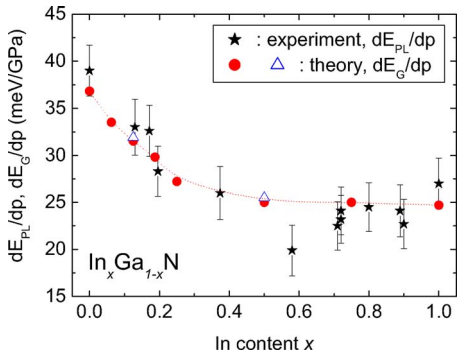

FIG. 5. (Color online) Dependence of the measured values of dE_{PL}/dp on In content in combination with the theoretical dependence of dE_G/dp on In content (filled red dots) obtained from the approach discussed in Sec. II A. Two different theoretical points at $x=0.125$ and $x=0.5$ (open blue triangles) correspond to different configurations of In atoms in a supercell. The experimental point concerning GaN is taken from Ref. 18.

of hydrostatic pressure show a very weak pressure shift of the PL bands of ~6–8 meV/GPa, which is very low both in comparison with the pressure-induced band gap shift as determined by absorption measurements (~30 meV/GPa) (Ref. 19) and compared to the present theoretical and experimental results (Fig. 5). This was interpreted as evidence of a localized donor state in the radiative recombination mechanism of In-rich InGaN. However, studies of the pressure dependence of the PL energy performed by our group on $In_xGa_{1-x}N$ alloy samples (of higher structural quality) with $0.6<x<1.0$ (also included in Fig. 5 of the present work) led to the contradictory conclusion that band-to-band transitions determine the nature of radiative recombination in InGaN alloys.[22] As a small but relevant digression, please note the difference between the value of dE_{PL}/dp for InN in Ref. 22 (21.4 meV/GPa) and the present work (27.4 meV/GPa). This value was corrected in regard to the recent finding that the value of dE_{PL}/dp is significantly lowered with respect to dE_G/dp in InN in the presence of large electron concentrations.[8] As mentioned in the Introduction, this effect is related to band filling effects in combination with the increase of the electron effective mass m^* with pressure. In view of their larger band gap energies, this effect can be expected to be much less pronounced in ternary InGaN alloys. In fact, it was demonstrated to be absent in the case of $In_{0.7}Ga_{0.3}N$.[23]

Furthermore, the agreement in Fig. 5 between the presented experimental results concerning dE_{PL}/dp and the theoretical curve of dE_G/dp produced via an *ab initio* approach implies that the hydrostatic pressure dependence of PL measurements can be used to quantify changes of the band gap of the InGaN ternary alloy under pressure. The disorder-related Stokes shift in InGaN, clearly observable in Fig. 2, is not large enough to cause a significant difference between dE_{PL}/dp and dE_G/dp. It should be added here that the reported experimental errors on dE_{PL}/dp are typical and cannot be expected to be improved much. This information is relevant for the correct analysis of pressure measurements. Indeed, as was mentioned in Sec. I, in the case of InGaN there exist several mechanisms which significantly reduce dE_{PL}/dp with respect to dE_G/dp. We conclude that the disorder-related Stokes shift is not one of those.

Next, we discuss the nature of the observed dependence of dE_G/dp on In content in InGaN. To begin with, the observed strong bowing of dE_G/dp versus In content can be attributed to either the absolute volume deformation potential of the band gap, $dE_G/d\ln V$, where V represents the volume, or to the bulk modulus B, which is defined as $dp/d\ln V$. The calculated values of the bulk moduli are 198 GPa for GaN and 148 GPa for InN with their pressure derivatives equal to 4.0 and 4.3, respectively. The values of the bulk moduli change linearly between GaN and InN. Similar results were obtained recently by pseudopotential calculations[24] [B(GaN)=200.6 GPa, B(InN)=145.6 GPa, and also linear dependence on In composition].

In Fig. 6 we plot the deformation potential of the band gap $a_G=dE_G/d\ln V$ as a function of indium composition x. We can see that the a_G curve essentially consists of two approximately linear sections, one at low x with a large slope

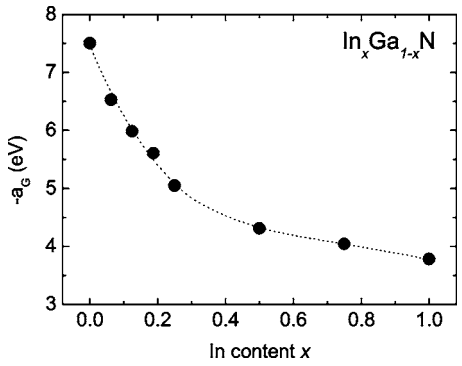

FIG. 6. Theoretical dependence of $a_G = dE_G/d \ln V$ in $In_xGa_{1-x}N$ on In content x.

and one for $x > 0.4$ with a much smaller slope corresponding to the "flat part" of the changes of dE_G/dp with x in Fig. 5. The effect of the In-content-dependent bulk modulus causes the two curves in Figs. 5 and 6 to differ in shape, but for both pressure and volume coefficients of the band gap two regions with different character of the x dependence are observed.

We have not found the reason why we observe two regions with different evolution of dE_G/dp versus In content: for $x < 0.4$, dE_G/dp decreases with increasing In content, whereas for higher x and up to InN dE_G/dp remains nearly constant. One can speculate that the former behavior may have some relation to the increase of valence band (VB) width due to (hybridization) admixture of In p-states to p-p bonding states,[5] which form the VB maximum (VBM) and are realized in GaN by N-anion and Ga-cation p-states. This anomalous behavior of the VBM was found earlier for In contents of $x = 0.10-0.25$.[5] A related effect can be found in the works of Bellaiche *et al.*[25] and Lee and Wang,[26] in which a nonlinear evolution of the gap with In content was found. For example, the calculations presented in Ref. 25 show for very low concentrations a strong admixture of In states and a hole localization. The admixture of the semi-core d-states of In- and Ga-cations represent another possible contribution to the sensitivity of VBM to pressure. This mechanism is described by the p-d coupling effect, which has been discussed on several occasions, for example in Refs. 21 and 27–30. The fact that for $x > 0.4$ no significant changes of dE_G/dp can be observed, in spite of considerable changes of both lattice constant and the band gap itself, remains to be clarified.

V. SUMMARY

Hydrostatic pressure-dependent measurements of the PL of $In_xGa_{1-x}N$ epilayers for the whole range of ternary alloys from GaN to InN were reported in conjunction with theoretical calculations of the InGaN band gap energy changes under pressure. Both experimental and theoretical results show pronounced bowing of the pressure coefficient, with a nearly constant value of about 25 meV/GPa for $In_xGa_{1-x}N$ epilayers with $x > 0.4$ and a relatively steep dependence for $x < 0.4$. As argued before in Ref. 22, the high values of the observed dE_{PL}/dp with respect to the expected significantly lower value in the case of recombination via localized donor states confirm the band-to-band character of radiative recombination in InGaN alloys.

Furthermore, the good agreement between the experimentally determined dE_{PL}/dp of $In_xGa_{1-x}N$ and the theoretical curve of dE_G/dp versus x indicates that the hydrostatic pressure dependence of PL measurements can be used to quantify changes of the band gap of the InGaN ternary alloy under pressure, demonstrating that the disorder-related Stokes shift in InGaN is not sufficient to cause a significant difference between dE_{PL}/dp and dE_G/dp. This information is highly relevant for the correct analysis of pressure measurements.

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